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# ELECTRONIC STRUCTURE OF STRAINED $Si_n/Ge_n(001)$ SUPERLATTICES

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Using the empirical tight binding method we have investigated the electronic properties of the $Si_n/Ge_n(001)$ strained superlattices as a function of the superlattice periodicity and the band misfit. For $n \geq 4$ we have found that first and second conduction band states are localized in Si. The hole states localized in Ge appear for $n \geq 4$. The difference between the direct and indirect band gaps is reduced from 2.01 eV for bulk Si to 0.01 eV for $n$=6 which can be considered to be quasi-direct. For the cases $n$=6 and $n$=8, the band gap might become direct for large values of band misfit.

Advances in molecular beam epitaxy have made the growth of the dislocation-free, strained-layer superlattices involving thin layers of semiconductors with large lattice mismatch possible[1]. In the $Si/Si_{1-x}Ge_x$ system grown on the $Si(001)$ substrate the lattice mismatch is completely accommodated by the uniform lattice strain in the commensurate $Si_{1-x}Ge_x$ layers. The layers parallel to the interface preserve the registry of the Si substrate, while the lattice constant in the perpendicular direction expands resulting in a tetragonal distortion. Since the energy barrier associated with reordering of atoms is too high, many defect-free commensurate layers can grow before the accumulated strain energy is relaxed by the generation of the misfit dislocations. The number of grown layers decreases with increasing $x$ (or Ge content in the alloy)[2].

Recently, the growth of the pure Ge upto six layers restricted to the $Si(001)$ surface unit cell have been achieved[3]. Most importantly, novel electronic properties of these strained $Si_n/Ge_n(001)$ superlattices have been reported[3,4,5] offering new device applications. For example Pearsall et al.[3] observed direct optical transitions at 0.76, 1.25 and 2.31 eV which were found neither in the constituent crystals ( i.e. Si and Ge ), nor in the $Si_{0.5}Ge_{0.5}$ alloy. It is hoped that the well developed Si technology will be used in optoelectronics, especially in laser applications.

We have investigated the electronic structure of the strained $Si_n/Ge_n(001)$ superlattices for $n$ ranging from 1 to 8. This paper presents our results providing an understanding of the effect of the superlattice periodicity on the electronic properties. The strained superlattices are constructed by taking Si atoms in their ideal positions, and by using the lattice constant of Si for the lateral lattice constant of the supercell. The separation of the $Si(001)$ and $Ge(001)$ layers at the interface, and the interlayer distance in the Ge site are obtained from the self-consistent field (SCF) pseudopotential calculations[4,5]. The structural parameters relevant to our study, and the superlattice Brillouin zone (SLBZ) are shown in Fig. 1 . In the same figure the relation between the symmetry points of the parent crystal BZ and that of the SLBZ, i.e. zone folding for the $Si_8(001)$ superstructure is also shown.

The purpose of the present work is to reveal how the electronic properties depend on the superlattice periodicity, rather than an accurate calculation of the band gap. Therefore, the electronic band structures are obtained by using the empirical tight binding (ETB) method. In fact an accurate calculation of the band gap by using an SCF-method within the local density functional theory seems to be a distant goal. On the other hand, a great care has to be exercised on the following points to obtain reliable results from the ETB calcula-

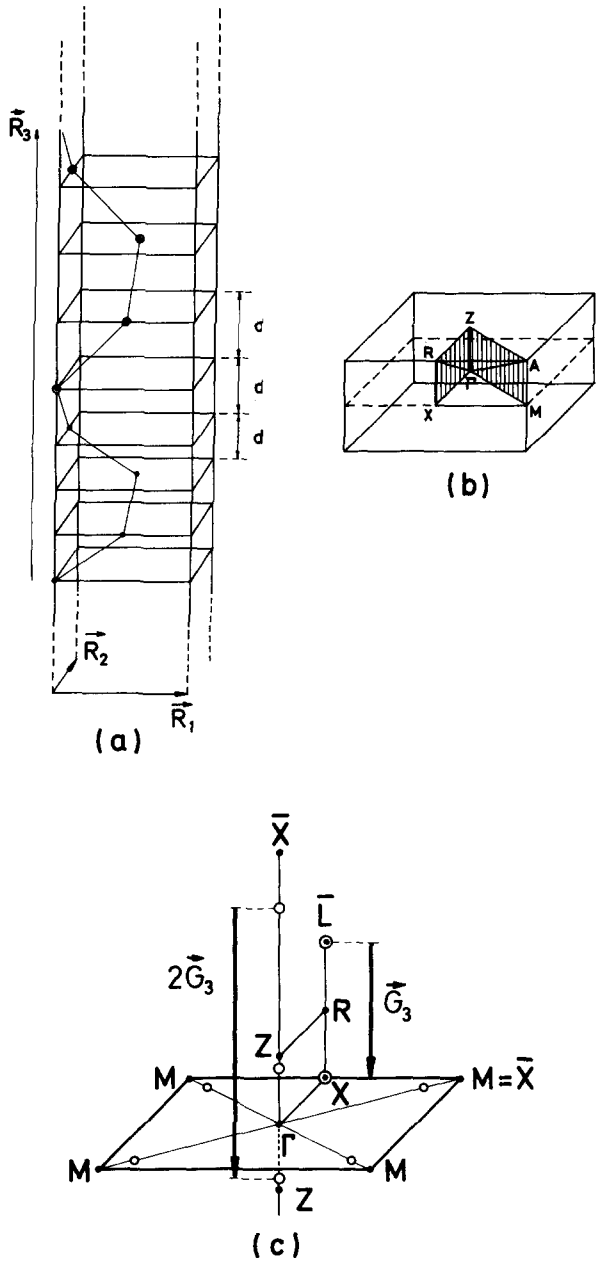


Fig.1. (a) Unit cell of the $Si_n/Ge_n(001)$ strained superlattice, with dots and dotted circles representing the Si and Ge atoms, respectively. The lateral lattice constants $R_1$ and $R_2$ are 5.43 Å/$\sqrt{2}$, the perpendicular lattice constant $R_3$ ( // [001] direction) changes according to $n$. Interlayer distances are $d_1$=5.43 Å/4, $d_2$=(5.43+5.65) Å/8 and $d_3$=5.82 Å/4. Lattice constants of bulk Si and Ge are taken to be 5.43 Å and 5.65 Å , respectively.(b) The corresponding Superlattice Brillouin Zone (SLZB). The width of Γ–Z decreases with increasing $n$. (c) The zone folding for the X- and L-points of the fcc BZ onto the SLZB. To avoid the confusion the X and L symmetry points of the fcc BZ are shown with bars.

tions for a system consisting of two different crystals: (i) The set of the energy parameters: We have used the energy parameters which are capable of yielding fairly good conduction bands, and which were proven to be successful in many previous applications[6]. (ii) The effect of the strain on the energy parameters: In the pseudomorphic Si/Ge system the Si–Ge and Ge–Ge interatomic distances, $d$, deviate from their ideal values because of the strain imposed by the lattice mismatch. This effect is taken into account by the $d^{-2}$ scaling[7,8] of the energy parameters. (iii) The band discontinuity: The energy of the valence band maximum, and also the average value of the crystal potential in two sublattice crystals (Si and Ge) are different[9]. This is the origin of the natural band lineup. Furthermore, to attain a common Fermi level, charge is normally transferred from one sublattice, to the adjacent one. The transferred charge creates a dipole field, which in turn affects the natural band lineup. While the dipole field induced by the transfer of charge, and thus the band discontinuity at the valence band, $\Delta E_v$, is directly obtainable by the SCF methods, this has to be implemented in the ETB calculations by shifting the self-energies, $\Delta E = < \phi_i(r) \mid H \mid \phi_i(r) >$, of Ge orbitals. We have examined the effect of the band lineup on the direct and indirect band gaps by calculating the electronic structure of $Si_n/Ge_n(001)$ for $\Delta E$ ranging from −1.0 eV to 1.5 eV.

The ordering of the gaps of $Si_4/Ge_4(001)$ relevant to our study is unaltered for $-0.9 < \Delta E < 0.25$ eV. In this energy range the states of Ge at the L-points of the BZ (which is folded near the X-points of the SLBZ) dominate the minimum of the conduction band. However, the ordering changes in the region $0.25 < \Delta E < 1.5$ eV several times. Beyond $\Delta E \geq 0.5$ eV the minimum occurs at the Z-point. Because of the size effect, and the Si–Ge interaction at the interface $\Delta E$ is not identical with $\Delta E_v$. In the rest of this study we used the values of $\Delta E$ which incorporates the values calculated by the SCF–pseudopotential method[4].

To reveal the effect of the superlattice formation on the electronic structure, we present the bands of $Si_8(001)$ superstructure in Fig. 2a. The bands of the strained $Ge_8(001)$ superstructure ( in which the lateral lattice constants $R_1$=$R_2$ are taken to be equal to that of the ideal Si, but interlayer distance, $d_3$, is expanded to accomodate the lateral strain ) are shown in Fig. 2b.

Silicon crystal has six minima along the Δ–direction of BZ denoted by the Δ*–states. The resulting experimental band gap is indirect and 1.1 eV. The direct band gap is large, and the energy difference between the direct and indirect band gap, $\Delta_{di}$, is ~2 eV. Also Ge is an indirect band gap semiconductor, except that the conduction band minima occur at the eight L-points of BZ. By forming a $Si_4/Ge_4(001)$ superlattice the effect of the zone folding[10], the lattice strain and the band lineup are combined in the electronic structure. Because of the tetragonal supercell

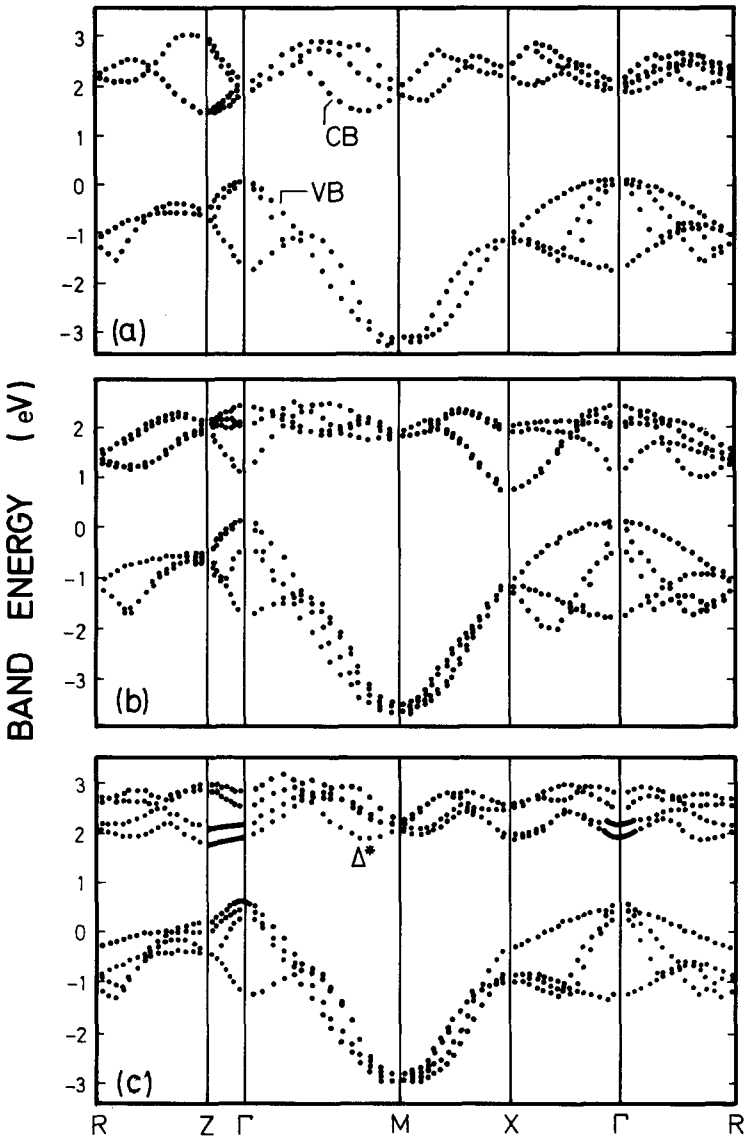


Fig.2. Energy bands for (a) $Si_8$(001) superstructure (b) $Ge_8$(001) strained superstructure restricted to $Si$(001) surface unit cell and (c) the $Si_4/Ge_4$(001) strained superlattice restricted to $Si$(001) surface unit cell. ($\Delta E$ = 0.84 eV.)

of $Si_8$(001) the bands with $\vec{k}$//[001] are folded along the ΓZ-direction of SLBZ. In addition to four minima ($\Delta^*$) along the ΓM-direction, the remaining two minima appear near the Z-point. The important effect of the band folding is that $\Delta_{di}$ is decreased from ~2 eV to 0.4 eV. Bands of $Ge_8$(001) experience similar foldings, and thus the minima of the conduction band occur at the X-point of SLBZ. Because of the tetragonal strain the valence bands, which are degenerate at Γ, are split and the energy of the highest state rises. The calculated value of the band splitting (0.59 eV) is in fair agreement with those calculated by the SCF-pseudopotential method[4,11]. The lowest and unfolded conduction band state at Γ also rises the net effect of the strain being the increase of the indirect band gap[11].

Upon the formation of the $Si_4/Ge_4$(001) superlattice the electronic state of the strained Ge-sublattice has to rise relative to that of the Si-sublattice. A state in one sublattice can match to the state in the adjacent one, as long as their momenta and energies are conserved. If their energies are different, the lower energy state is generally confined in its sublattice. The effective

masses along the superlattice axis, and the size of the quantum well may influence the confinment. Also, owing to the coupling between the sublattices of the same kind the bands of the confined states along $\vec{k}$//[001] direction may have a dispersion. The energy band picture of the $Si_4/Ge_4$(001) superlattice presented in Fig. 2c illustrates these effects.

The striking effect of the superlattice structure can be seen in Fig. 2c by the minizone formation along the ΓZ-direction in the conduction band clearly. While the conduction bands of the Ge and Si superstructures in Fig. 2a and 2b have significant dispersion, and states are uniformly distributed over the unit cell for $\vec{k}$//[001], the corresponding bands of $Si_4/Ge_4$(001) are rather flat. The first and second conduction bands along the ΓZ-direction have 80% Si-orbital character displaying a confinement in the Si-region, but rather low weight in the Ge-side. These flat bands have a parabolic dispersion for $\vec{k}$//[001] plane, which is characteristic for a 2D-electron system. Since the minimum of the conduction band occurs at the Z-point the $Si_4/Ge_4$(001) superlattice is an indirect band gap semiconductor. The indirect band gap is calculated to be 1.15 eV. The $\Delta_{di}$ is equal to the dispersion of the first conduction band along Γ–Z, and is only 0.15 eV. For $-0.5 < \Delta E < 0.5$ eV, $\Delta_{di}$ is strongly dependent on $\Delta E$. The value of the band offset used in this study is beyond this range, at which $\Delta_{di}$ is not dependent on $\Delta E$, however. Note that $\Delta_{di}$ being 0.34 and 2.01 eV in the bulk Ge and Si, changed to 0.4 and 0.46 eV, respectively upon the formation of strained $Ge_8$(001) and $Si_8$(001) superstructures. Evidently, the reduction of $\Delta_{di}$ in $Si_4/Ge_4$(001) is even more dramatic. The states of the third conduction band are delocalized and have comparable charges in both Si- and Ge-regions, but the states of the fourth band are mainly localized in the Ge-region. Furthermore, Fig. 3 shows how the localization of the conduction and valence band states at certain symmetry points of the SLZB depends on $\Delta E$.

The highest valence band states at the Γ-point, as well as along the ΓZ-direction originate from the Ge-orbitals, implying the fact that holes in this strained superlattice are confined in the Ge-region. Taking only the ΓZ-direction into account, the confinement of the states (electrons being localized in the Si region and holes in the Ge-region) displays a type II-staggered band discontinuity, which complies with the band lineup implemented in our model, and with the experimental results as well[12]. It is interesting to note that the present results are in agreement with those obtained by the *ab-initio* calculations, except the location of the conduction band minimum. For instance the SCF-pseudopotential calculations[11] yield that the lowest conduction band state is an extended state, and occurs at the Δ*-point, 0.08 eV below the state at the Z-point. In the present study the Δ* state becomes confined only for $\Delta E > 0.6$ eV. The transitions from the extended to confined state at the M-point is a discontinuous function of $\Delta E$.

Another interesting feature of our results which deserves a comment is that a heterostructure with such a small superlattice periodicity can support confined states (or localized states). Certainly, the band dis-

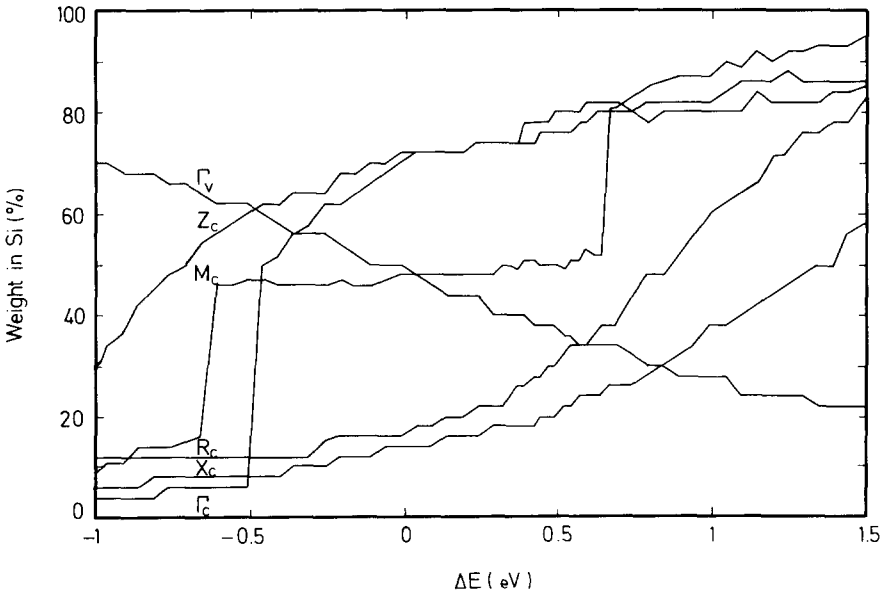


Fig.3. Localization (weight in Si-sublattice) of the conduction and valence band states of $Si_4/Ge_4$(001) as a function of $\Delta E$.

continuity in a heterostructure is a macroscopic property, and is meaningful only when two sides (here Si and Ge sublattices) have considerable thicknesses (perhaps 10–15 atomic layers), where the size effect is insignificant. For example, the $Si_n/Ge_n(001)$ structure for $n$=1, or 2 is a crystal rather than a heterostructure, because the bulk-like regions are merged in the interface[13]. The present results, as well as the recent SCF-pseudopotential calculations[4,5,11] reveal that the bulk-like properties at both sides begin to recover for $n \geq 3$, however, not quite enough to be compared with the Kronig-Penney type models[13].

Having discussed the strained superlattices for $n = 4$, let us consider the cases for $n = 3$ and $n = 6$ to explore the effect of the superlattice periodicity. For $n = 3$ the quantum well states are not fully developed, and thus appeared as interface states. Upon increasing $n$ to 6 the difference of energy between the direct and indirect band gaps reduces to 0.01 eV. The lowest conduction band minima occur at the Z-point. Along the ΓZ-direction and at the Γ-point the localization of the conduction band states in Si are stronger than that for $n$=4. The dispersion of the valence bands along the ΓZ-direction is reduced, and their localization in the Ge-region is enhanced. Furthermore, the number of hole states confined in Ge increases from one to two upon increasing $n$ from 4 to 6. By going from $n$=6 to $n$=8 the localization of the quantum well states increases and the indirect band gap decreases.

The important results obtained from this study of the pseudomorphic $Si_n/Ge_n(001)$ superlattices can be summarized as follows: (i) For $n \leq 3$ the superlattices do not allow any quantum well structure, and the states are localized therein. These localized states appear as interface states. For $n \geq 4$ the superlattices can support the electron confined states. Increasing $n$ (or increasing sublattice thickness) decreases the coupling between quantum wells, and thus increases the localization of these states. First and second conduction band states along Γ–Z are localized in the Si sublattice, which originate from the lowest conduction band along the Δ direction of the BZ. However, the state near $\Delta^*$ has small effective mass for $\vec{k}//(001)$ plane, therefore the lowest conduction band states along Γ–M can be localized only for large $\Delta E$. This is a manifestation of the size effect. (ii) While only one hole state is confined in the Ge–sublattice for $n$=4, both the number and localization of the confined hole states increase for $n$=6 and $n$=8. (iii) For the superlattice periodicities studied here ($n$=3,4,6 and 8) the band gap is found to be indirect. However, the difference of energy between the direct and indirect band gap reduces from 0.15 eV for $n = 4$ to 0.01 eV for $n = 6$. In view of this small difference one can assume that the band gap is quasi-direct[14]. In fact, for larger values of $\Delta E$ ($> 0.57$ eV for $n$=6 and $> 0.69$ eV for $n$=8) the band gap becomes direct. (iv) The energies of the indirect band gap are 1.46, 1.15, 1.06 and 0.92 eV for $n$= 3,4,6,8, respectively. Since the lowest conduction band state at Γ is a confined state, its energy has an inverse proportionality with $n$, the exponent being between 1 and 2. (v) No direct band gap as small as 0.76 eV is found to support the direct transition obtained from the recent electroreflectance spectroscopy[3]. However, such a small direct band gap might be possible for $n$=6 with band offset as big as 1.2 eV. As compared to observed direct transitions[3] ($0.76 \mp 0.13, 1.25 \mp 0.13$, and $2.31 \mp 0.12$ eV) we found the direct transitions at Γ of 1.30, 1.55, and 1.91 eV for $n$=4.

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